Summer Program FGV/EMAp 2019

Introduction to Machine Learning with Python

PRINCIPAL COMPONENT ANALYSIS

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Principal Component Analysis

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Lets so make a quick review of eigenvectors, eigenvalues, and covatiance matrices.

Eigenvectors and Eigenvalues

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- $\lambda \in \mathbb{R}$ and $\mathbf{u} \in \mathbb{R}^d$ (no complex numbers involved).
- The eigenvectors are orthogonal

$$\mathbf{u}_i^\top \mathbf{u}_j = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{otherwise} \end{cases}$$

(assuming $\|\mathbf{u}_i\| = 1$)

Symmetric Matrices

$\mathbf{A}$ symmetric with distinct eigenvalues λ_i.

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Spectral Decomposition of a Symmetric Matrix

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^\top$$

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$$f(x_1, x_2) = [x_1\, x_2] \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = x_1^2 + x_2^2$$

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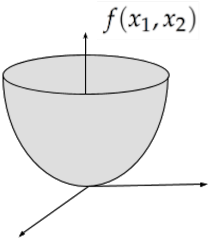

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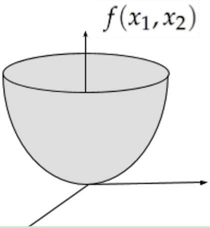

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$$\max_{\|\mathbf{x}\|=1} \{f(\mathbf{x})\} = \mathbf{u}_1^\top \mathbf{A}\mathbf{u}_1 = \lambda_1$$

$$\min_{\|\mathbf{x}\|=1} \{f(\mathbf{x})\} = \mathbf{u}_d^\top \mathbf{A}\mathbf{u}_d = \lambda_d$$

$(\lambda_1, \mathbf{u}_1)$ and $(\lambda_d, \mathbf{u}_d)$ are the larger and smaller eigenpair.

Covariance Matrix

Let $\mathbf{x}_i = [x_{1i}, \ldots, x_{di}]^\top$, $\mathbf{x}_j = [x_{1j}, \ldots, x_{dj}]^\top$

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The covariance between $\mathbf{x}_i$ and $\mathbf{x}_j$ is given by

$$cov(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{d-1} \sum_{s=1}^{d} (x_{si} - \overline{x}_i)(x_{sj} - \overline{x}_j)$$

where $\overline{x}_i = \frac{1}{d} \sum_s x_{si}$ and $\overline{x}_j = \frac{1}{d} \sum_s x_{sj}$

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If we assume $\mathbf{x}_i$ and $\mathbf{x}_j$ centered, that is, $\overline{x}_i = 0$ and $\overline{x}_j = 0$

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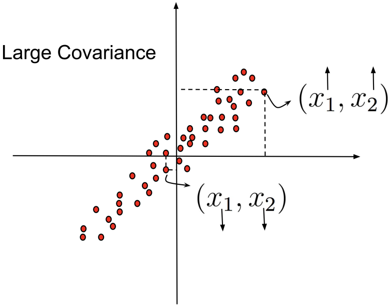

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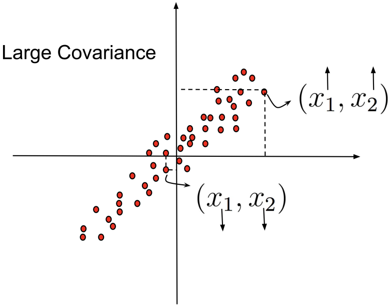

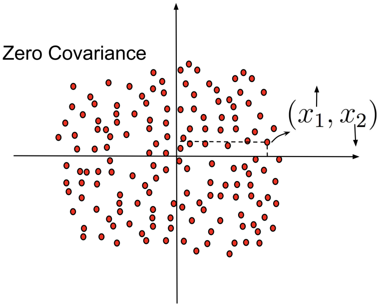

Covariance Matrix

Assuming $\mathbf{x}_i$, $i = 1, \ldots, n$ a centered set of data instances (points in $\mathbb{R}^d$) arranged in a data matrix $\mathbf{X}$:

$$\mathbf{X} = \begin{bmatrix} | & | & & | \\ \mathbf{x}_1 & \mathbf{x}_2 & \ldots & \mathbf{x}_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \ldots & x_{1n} \\ x_{21} & x_{22} & \ldots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{d1} & x_{d2} & \ldots & x_{dn} \end{bmatrix} \tag{1}$$

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The covariance matrix of $\mathbf{X}$ is the symmetric matrix:

$$\frac{1}{n-1}\mathbf{X}\mathbf{X}^\top = \begin{bmatrix} \boxed{cov(x_{1:}, x_{1:})} & cov(x_{1:}, x_{2:}) & \ldots & cov(x_{1:}, x_{d:}) \\ cov(x_{2:}, x_{1:}) & \boxed{cov(x_{2:}, x_{2:})} & \ldots & cov(x_{2:}, x_{d:}) \\ \vdots & \vdots & \ddots & \vdots \\ cov(x_{d:}, x_{1:}) & cov(x_{d:}, x_{2:}) & \ldots & \boxed{cov(x_{d:}, x_{d:})} \end{bmatrix}$$

Variances are in the main diagonal

Principal Components: getting some intuition

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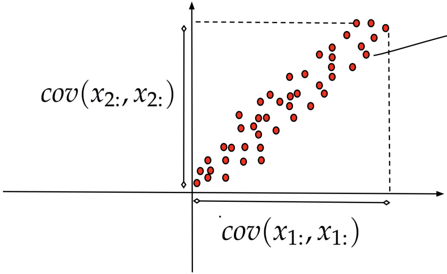

$$\mathbf{X}\mathbf{X}^\top = \begin{bmatrix} cov(x_{1:}, x_{1:}) & cov(x_{1:}, x_{2:}) \\ cov(x_{2:}, x_{1:}) & cov(x_{2:}, x_{2:}) \end{bmatrix}$$

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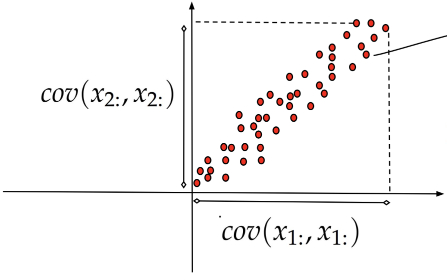

not zero

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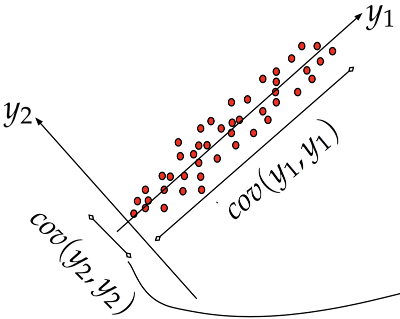

$$\mathbf{Y}\mathbf{Y}^\top = \begin{bmatrix} cov(y_1, y_1) & 0 \\ 0 & cov(y_2, y_2) \end{bmatrix}$$

close to zero

Principal Components

The idea of PCA is to find a new basis to write the data so as to vanish the covariance between distinct attributes.

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Mathematically, we are looking for a change of basis matrix $\mathbf{P}$ such that

$$\mathbf{Y} = \mathbf{P}\mathbf{X} \Longrightarrow \mathbf{Y}\mathbf{Y}^\top = \mathbf{D}$$

where $\mathbf{D}$ is a diagonal matrix with diagonal elements corresponding to the variance of each coordinate (attribute).

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- we will be able to reduce the dimension of the data without loosing relevant information.

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Reminder

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Moreover,

$$\mathbf{u}_1^\top \mathbf{X}\mathbf{X}^\top \mathbf{u}_1 = \lambda_1 \text{ (maximum of the quadratic form)}$$

$$\mathbf{u}_d^\top \mathbf{X}\mathbf{X}^\top \mathbf{u}_d = \lambda_d \text{ (minimum of the quadratic form)}$$

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$\mathbf{u}_1$ is the direction that maximizes the variance and $\mathbf{u}_d$ the direction that minimizes the variance.

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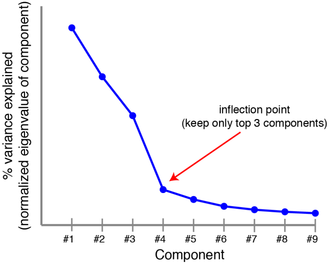
We can reconstruct "noise-free" data by $\hat{\mathbf{X}} = \mathbf{U}\hat{\mathbf{Y}}$

$$\hat{\mathbf{Y}} = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1n} \\ & & \vdots & \\ y_{k1} & y_{k2} & \cdots & y_{kn} \\ 0 & 0 & \cdots & 0 \\ & & \vdots & \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$



$$T = \frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$$